

Comment on “Periodic wave functions and number of extended states in random dimer systems”

In a recent report,¹ Huang *et al.* studied numerically the electronic properties of a random dimer model (RDM) and found extended periodic wave functions near the critical energies. They also claimed that the number of extended states is proportional to \sqrt{N} , where N is the size of the system, which is consistent with previous results.

(i) There are *no* periodic wave functions in the RDM. Indeed, even at the critical energies it was shown previously² that the wave functions have a constant norm but the phases are random. Essentially the wave function is $\psi_i = e^{i\theta_i}$, where θ_i is random. This does, however, lead to a constant envelope. We define the envelope as the ensemble of curves which include all possible values of the random wave function. In this point we present the analytical derivation against the main result presented in Ref. 1 and show that the envelope (and *not* the wavefunction itself) is periodic near the critical energies as long as the localization length exceeds the size of the system.

The RDM can be analyzed in terms of the product of the following two transfer matrices³

$$T_A = \begin{pmatrix} E - V_A & -1 \\ 1 & 0 \end{pmatrix}^2, \quad T_B = \begin{pmatrix} E - V_B & -1 \\ 1 & 0 \end{pmatrix}^2. \quad (1)$$

They reduce to the negative identity matrix when $E = V_A$ or $E = V_B$ (critical energies), which means that T_A and T_B commute. Close to the critical energy, i.e., when $\Delta E = E - V_A$ is small, the commutator $[T_A, T_B] = O(\Delta E)$, as opposed to the case without the dimer condition, where the commutator is always of order 1. The total system is described by a random mixture of the products of the transfer matrices T_A and T_B , thus $T = \prod_i T_A^{n_i} T_B^{m_i}$, where n_i and m_i are random. Therefore the total product is $T = T_A^n T_B^m + (N/4)O(\Delta E)$, where $n = \sum_i n_i$, $m = \sum_i m_i$ and $N = 2(n+m)$. This clearly demonstrates that the solution is equivalent to the system with

$$T = (-1)^n T_B^m, \quad (2)$$

as long as N is smaller than $1/\Delta E$.

The main result here is that the envelope of Eq. (2) reproduces all the numerical figures of Ref. 1. Indeed Huang *et al.* studied numerically two cases:

(a) $V_A = -1$, $V_B = 1$ and $E = -1 + \Delta E$. As the envelope can be obtained from the solution of T_B^m , the corresponding wave-functions can be written as $\psi_i \sim \cos(ki)$, where $E - V_B = 2 \cos(k)$. To first order in ΔE we obtain $k \simeq \pi - \sqrt{\Delta E/2}$. From this follows trivially that the general solution has periodic solutions for $2m\sqrt{\Delta E/2} = \pi p$, where p is an integer. This leads to $\Delta E = 2\pi^2 p^2/(N/2)^2$, where $N/2$ is the number of dimers when they are equally distributed.

(b) $V_A = -0.5$, $V_B = 0.5$ and $E - V_B = -1 + \Delta E$. In this case we obtain $k \simeq 2\pi/3 - \sqrt{3}\Delta E/2$ and $\Delta E = 2\pi p/\sqrt{3}(N/2)$.

In both cases (a) and (b) we obtain the same dependences as in Ref. 1.

(ii) The use of the inverse participation ratio (IPR)

$$\text{IPR} = N \sum_{j=1}^N |\psi_j|^4, \quad (3)$$

where ψ_j is the normalized wave function at site j , is very ambiguous and a complete multifractal analysis is required in determining the extension of the wave function.⁴ We can indeed construct delocalized wavefunctions with arbitrary IPR. For instance, we can consider the following periodic (normalized) wave function $\psi_j^2 = T/N$ if $j/T = \text{integer}$ and $\psi_j^2 = 0$ otherwise, where the period T is an integer ($T < N$) then from (3), we obtain $\text{IPR} = T$. In this way we have a set of delocalized states with arbitrary IPR.

(iii) The number of extended states is proportional to \sqrt{N} , which means that the relative number of extended states tends to zero as $1/\sqrt{N}$, therefore the delocalization properties are important only in small systems.⁵

In conclusion, there are *no* periodic wave-functions in the RDM but close to the critical energies there exist periodic envelopes. These envelopes are given by the non-disordered properties of the system.

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